

wwPDB X-ray Structure Validation Summary Report (i)

Sep 27, 2022 – 10:50 am BST

PDB ID : 7ZML

Title: Crystal structure of human RECQL5 helicase APO form in complex with

engineered nanobody (Gluebody) G1-001

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Deposited on : 2022-04-19

Resolution : 2.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.31.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0267$

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

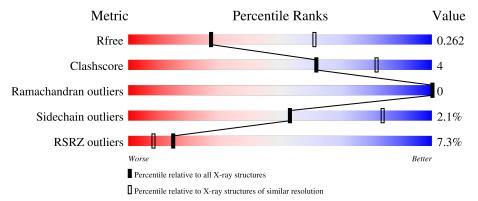
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
			3%		
1	A	445	85%	14%	•
			6%		
1	В	445	87%	11%	•
			8%		
1	С	445	86%	13%	•
			17%		
1	D	445	85%	14%	
			3%		
2	E	132	88%	7% •	•



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Mol	Chain	Length	Quality of chain		
2	F	132	8%	11%	-
2	G	132	86%	14%	-
2	K	132	88%	11%	-

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	502	-	-	X	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17730 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	Λ	441	Total	С	N	О	S	0	4	0
1	A	441	3452	2180	622	627	23	0	4	
1	В	441	Total	С	N	О	S	0	1	0
1	Ъ	441	3409	2155	605	626	23	0	4	0
1	С	441	Total	С	N	О	S	0	5	0
1		441	3432	2169	612	628	23	0	9	
1	D	440	Total	С	N	О	S	0	5	0
1	ע	440	3452	2180	623	626	23	U	J	U

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	-	expression tag	UNP O94762
A	10	MET	-	expression tag	UNP O94762
В	9	SER	-	expression tag	UNP O94762
В	10	MET	-	expression tag	UNP O94762
С	9	SER	-	expression tag	UNP O94762
С	10	MET	-	expression tag	UNP O94762
D	9	SER	-	expression tag	UNP O94762
D	10	MET	-	expression tag	UNP O94762

• Molecule 2 is a protein called Gluebody G1-001.

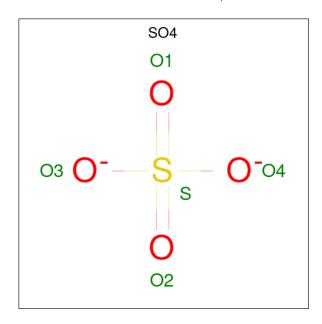
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	K	131	Total	С	N	О	S	0	0	0
2	11	131	996	623	169	200	4	0	U	U
2	E	128	Total	С	N	О	S	0	0	0
2	<u> </u>	120	965	599	166	196	4	0	0	U
2	F	130	Total	С	N	О	S	0	0	0
2	I'	150	985	614	168	199	4	0	U	U
2	G	131	Total	С	N	О	S	0	0	0
	G	191	996	623	169	200	4	U	U	U



• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	В	1	Total O S 5 4 1	0	0
4	С	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0



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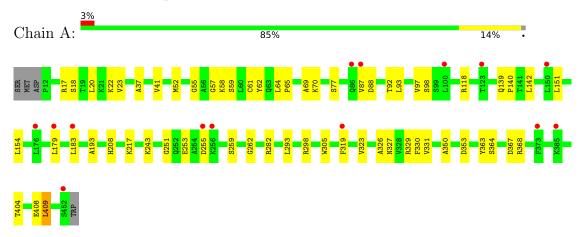
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	6	Total O 6 6	0	0
5	С	2	Total O 2 2	0	0
5	D	2	Total O 2 2	0	0
5	K	1	Total O 1 1	0	0
5	E	3	Total O 3 3	0	0
5	G	2	Total O 2 2	0	0



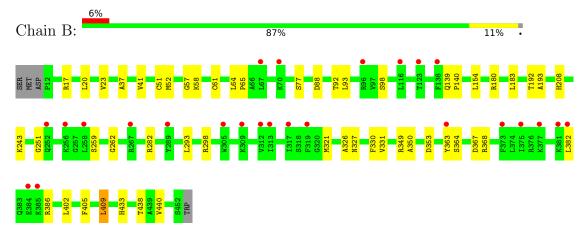
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

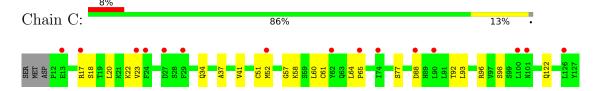
• Molecule 1: ATP-dependent DNA helicase Q5



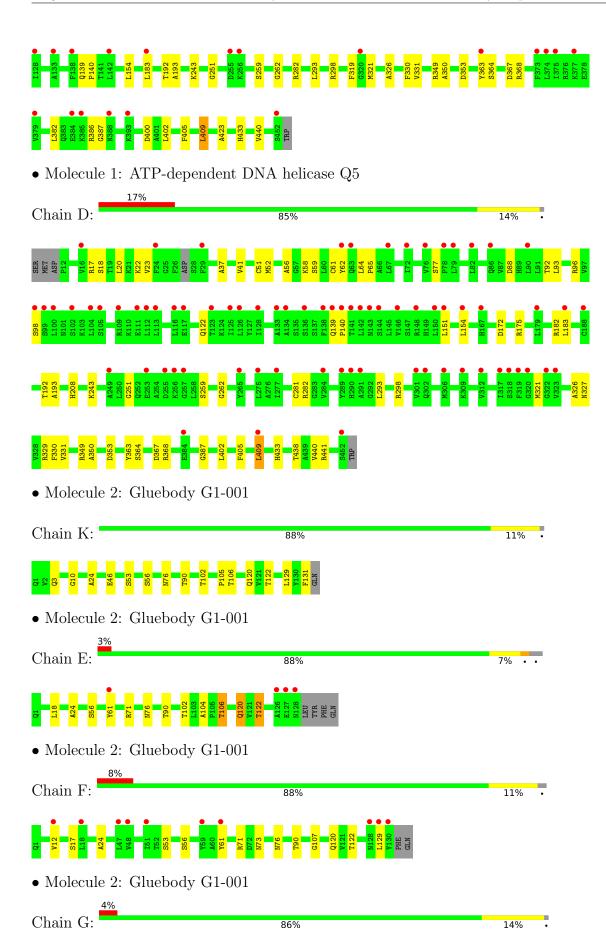
• Molecule 1: ATP-dependent DNA helicase Q5



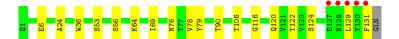
• Molecule 1: ATP-dependent DNA helicase Q5













4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	75.74Å 185.53Å 101.01Å	Donogitor
a, b, c, α , β , γ	90.00° 107.47° 90.00°	Depositor
Resolution (Å)	96.35 - 2.79	Depositor
Resolution (A)	96.35 - 2.79	EDS
% Data completeness	99.6 (96.35-2.79)	Depositor
(in resolution range)	99.6 (96.35-2.79)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.56 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.224 , 0.261	Depositor
R, R_{free}	0.227 , 0.262	DCC
R_{free} test set	3147 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ < L > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17730	wwPDB-VP
Average B, all atoms $(Å^2)$	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bo	ond angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.67	0/3528	0.84	0/4766
1	В	0.67	0/3504	0.81	0/4738
1	С	0.67	0/3525	0.81	0/4764
1	D	0.66	0/3526	0.80	0/4761
2	Е	0.67	0/983	0.87	1/1332 (0.1%)
2	F	0.67	0/1004	0.85	0/1361
2	G	0.67	0/1016	0.86	0/1377
2	K	0.68	0/1016	0.87	0/1377
All	All	0.67	0/18102	0.83	$1/24476 \ (0.0\%)$

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	${ m E}$	71	ARG	NE-CZ-NH2	-5.34	117.63	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3452	0	3484	37	0
1	В	3409	0	3399	31	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	3432	0	3439	31	0
1	D	3452	0	3481	36	0
2	Ε	965	0	918	5	0
2	F	985	0	938	6	0
2	G	996	0	947	13	0
2	K	996	0	947	8	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	2	0
4	В	5	0	0	1	0
4	С	5	0	0	1	0
4	D	5	0	0	0	0
5	A	3	0	0	1	0
5	В	6	0	0	0	0
5	С	2	0	0	0	0
5	D	2	0	0	0	0
5	Ε	3	0	0	0	0
5	G	2	0	0	0	0
5	K	1	0	0	0	0
All	All	17730	0	17553	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 156 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:D:243:LYS:HD3	1:D:282:ARG:HB3	1.69	0.74
1:A:142:LEU:CD2	1:A:179:LEU:HD11	2.18	0.73
1:B:208:HIS:ND1	1:D:387:GLY:HA3	2.06	0.70
1:D:52:MET:O	1:D:193:ALA:HA	1.92	0.69
2:E:90:THR:HG23	2:E:122:THR:HA	1.76	0.68

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	443/445 (100%)	431 (97%)	12 (3%)	0	100	100
1	В	443/445 (100%)	432 (98%)	11 (2%)	0	100	100
1	\mathbf{C}	444/445 (100%)	432 (97%)	12 (3%)	0	100	100
1	D	441/445 (99%)	428 (97%)	13 (3%)	0	100	100
2	E	126/132 (96%)	124 (98%)	2 (2%)	0	100	100
2	F	128/132 (97%)	126 (98%)	2 (2%)	0	100	100
2	G	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
2	K	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
All	All	2283/2308 (99%)	2223 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	369/373~(99%)	365 (99%)	4 (1%)	73 92
1	В	365/373~(98%)	361 (99%)	4 (1%)	73 92
1	C	368/373~(99%)	364 (99%)	4 (1%)	73 92
1	D	368/373~(99%)	363 (99%)	5 (1%)	67 90
2	E	$98/103\ (95\%)$	92 (94%)	6 (6%)	18 48
2	F	100/103~(97%)	95 (95%)	5 (5%)	24 56



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	101/103 (98%)	96 (95%)	5 (5%)	24 56
2	K	101/103 (98%)	95 (94%)	6 (6%)	19 49
All	All	1870/1904 (98%)	1831 (98%)	39 (2%)	53 84

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Е	122	THR
2	G	56	SER
2	F	12	VAL
2	F	120	GLN
2	G	106	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	208	HIS
1	D	101	ASN
2	F	3	GLN
1	D	285	ASN
2	K	3	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Trino	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	502	-	4,4,4	0.30	0	6,6,6	0.23	0
4	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.26	0
4	SO4	В	502	-	4,4,4	0.44	0	6,6,6	0.09	0
4	SO4	С	502	-	4,4,4	0.32	0	6,6,6	0.21	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	SO4	2	0
4	В	502	SO4	1	0
4	С	502	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	441/445 (99%)	0.11	14 (3%) 47 37	61, 93, 143, 230	0
1	В	441/445 (99%)	0.29	25 (5%) 23 15	65, 109, 177, 212	0
1	С	441/445 (99%)	0.35	34 (7%) 13 7	65, 113, 180, 206	0
1	D	440/445 (98%)	0.87	74 (16%) 1 1	76, 136, 211, 259	0
2	E	128/132 (96%)	0.19	4 (3%) 49 39	57, 83, 133, 210	0
2	F	130/132 (98%)	0.45	10 (7%) 13 7	55, 82, 131, 243	0
2	G	131/132 (99%)	0.06	5 (3%) 40 30	55, 78, 157, 169	0
2	K	131/132 (99%)	-0.05	0 100 100	58, 74, 105, 134	0
All	All	2283/2308 (98%)	0.35	166 (7%) 15 8	55, 103, 183, 259	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Е	128	ASN	20.7
1	D	100	LEU	9.7
1	С	320	GLY	9.6
2	F	130	TYR	9.5
2	G	131	PHE	8.4

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	SO4	D	502	5/5	0.86	0.12	130,160,175,187	0
4	SO4	С	502	5/5	0.90	0.11	101,123,142,150	0
3	ZN	A	501	1/1	0.96	0.18	101,101,101,101	0
4	SO4	A	502	5/5	0.96	0.14	73,76,115,120	0
3	ZN	D	501	1/1	0.97	0.12	146,146,146,146	0
4	SO4	В	502	5/5	0.98	0.15	93,103,115,124	0
3	ZN	С	501	1/1	0.99	0.17	102,102,102,102	0
3	ZN	В	501	1/1	1.00	0.20	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.

